

APPLIED CHEMISTRY DEPARTMENT
S. V. NATIONAL INSTITUTE OF TECHNOLOGY, SURAT
Ph.D. COMPREHENSIVE EXAMINATION SYLLABUS

INORGANIC CHEMISTRY

- **Main Group Elements:** Hydrides, halides, oxides, oxoacids, nitrides, sulfides – shapes and reactivity. Structure and bonding of boranes, carboranes, silicones, silicates. Allotropes of carbon. Acid-base concepts.
- ***d* – and *f*– block elements:** Coordination chemistry – structure and isomerism, theories of bonding (VBT, CFT, and MOT). Energy level diagrams in various crystal fields, CFSE, applications of CFT, Jahn-Teller distortion. Electronic spectra of transition metal complexes: spectroscopic term symbols, selection rules, Orgel diagrams, charge-transfer spectra. Magnetic properties of transition metal complexes. Lanthanides and Actinides: Electronic configuration and periodic properties
- **Organometallics:** 18-Electron rule; metal-alkyl, metal-carbonyl, metal-olefin and metallocenes. Types of organometallic reactions. Homogeneous catalysis - Hydrogenation, hydroformylation, acetic acid synthesis, metathesis and olefin oxidation. Heterogeneous catalysis - Fischer-Tropsch reaction, Ziegler-Natta polymerization.
- **Bioinorganic Chemistry:** Metalloenzymes containing magnesium, Molybdenum iron, cobalt, copper and zinc.
- **Solids:** Crystal systems and lattices, Miller planes, crystal packing, crystal defects, Bragg's law, ionic crystals, structures of AX, AX₂, ABX₃ type compounds, spinels and inverse spinels

ORGANIC CHEMISTRY

- **Stereochemistry and Reaction Mechanisms:** Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
Methods of determining reaction mechanisms through identification of products, intermediates and isotopic labeling. Nucleophilic and electrophilic substitution reactions (both aromatic and aliphatic). Addition reactions to carbon-carbon and carbon-heteroatom (N,O) multiple bonds. Elimination reactions. Reactive intermediates – carbocations, carbanions, carbenes, nitrenes, arynes and free radicals. Molecular rearrangements involving electron deficient atoms.
- **Organic Synthesis:** Synthesis, reactions, mechanisms and selectivity involving the following classes of compounds – arenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, esters, nitriles, halides, nitro compounds, amines and amides. Uses of Mg, Li and B based reagents in organic synthesis. Protection and deprotection of functional groups. Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers. Michael addition reaction.

PHYSICAL CHEMISTRY

- **Electrochemistry:** Types of electrochemical cells, cell reactions, e.m.f. and change in free energy, Nernst equation. Standard cells. Half-cells/electrodes, different types of electrodes. Standard electrode potential and principles of its determination. Types of concentration cells. Liquid junction potential. Glass electrode and determination of pH of a solution. Potentiometric titrations: acid-base and redox, electro chemical power sources; primary, secondary and fuel Cells, corrosion and inhibition of corrosion.
- **Equilibrium:** Laws of thermodynamics. Standard states. Thermochemistry. Thermodynamic functions and their relationships: Gibbs-Helmholtz and Maxwell relations, van't Hoff equation. Phase rule: Phase diagram of one component systems: CO₂, H₂O, S; Fractional distillation. Azeotropes and eutectics.
- **Chemical Kinetics:** Transition state theory: Eyring equation, thermodynamic aspects. Potential energy surfaces and classical trajectories. Elementary, parallel, opposing and consecutive reactions. Steady state approximation.
- **Surfaces and Interfaces:** Physisorption and chemisorption. Langmuir, Freundlich and BET isotherms. Physical chemistry of colloids, micelles and macromolecules.

ANALYTICAL CHEMISTRY

- **Instrumental Methods of Analysis:** UV-visible spectrophotometry, FT-IR, NMR and ESR spectroscopy, mass spectrometry, Fluorescence and atomic absorption spectrometry, Chromatography including GC, GC-MS, HPLC and LC-MS. Thermoanalytical and Electroanalytical techniques: Potentiometry. polarography, cyclic voltammetry
- **Material Characterization Techniques:** SEM, TEM and XRD.

INTERDISCIPLINARY TOPICS

- Nanoscience and Technology / Green Chemistry and Catalysis / Supramolecular Chemistry / Wastewater treatment / Solution Chemistry / Polymer Chemistry / Medicinal Chemistry / Quantum Chemistry / Materials and Biomaterials Chemistry

RECOMMENDED BOOKS

1. R. S. Drago, *Physical Methods in Inorganic Chemistry*, first edition, (1971), Affiliated East-West Press, New Delhi.
2. J. D. Lee, *Concise Inorganic Chemistry*, fourth edition ELBS, 1991.
3. A. I. Vogel, *Elementary Practical Organic Chemistry: Qualitative Organic Analysis*, second edition, Dorling Kindersley (India) Pvt. Ltd., Pearson Education, South Asia, 1997.
4. G. M. Barrow, *Physical Chemistry*, Tata McGraw Hill; New Delhi, 1996.
5. D. A. Skoog, F. J. Hoes, T. A. Nieman, *Principles of Instrumental Analysis*, fifth Edition, Saunders College Publishing, Philadelphia, 1998.
6. J. Clayden, S. Warren, N. Greeves, P. Wothers, *Organic Chemistry*, second edition, Oxford University Press, 2012.
7. M. B. Smith, J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, sixth edition, Wiley-Interscience, 2012.